

SUPPLEMENTAL INFORMATION

Supplemental Experimental Procedures

Protein production, purification, and crystallization. A cDNA encoding the full-length prM and ectodomain of E of ZIKV (strain H/PF/2013, residues 123-696, GenBank Accession KJ776791) was placed in the mammalian expression vector pFM1.2 (Mancia et al., 2004) downstream of a human IL-2 signal sequence peptide (MPLLLLLPLLWAGAL) and terminated with a hexahistidine affinity tag. The protein was expressed by transient transfection of Expi293F cells using HYPE-5 reagent (Oz Biosciences) in serum-free Expi293 medium (Thermo Fisher). Cell supernatants were harvested 72 h after transfection. The soluble E protein was recovered by capture on nickel agarose beads (Goldbio) and purified by passage over S200 Superdex. The protein storage buffer contained 25 mM HEPES-HCl pH 7.4, 150 mM NaCl, and 0.01% sodium azide at 4°C. A ZIKV quad-fusion-loop variant (ZIKV E-FL) was made by site-directed mutagenesis (T76A, Q77G, W101R, L107R, as numbered from the mature N-terminus). A cDNA encoding the full-length prM and ectodomain of E DENV-4 (residues 113-678 of strain H241, GenBank accession AY947539) was inserted into pFM1.2 vector for transient expression in Expi293F cells. WNV E ectodomain (residues 291-694 of strain New York 1999, GenBank accession YP001527877) was produced in bacteria and refolded as described previously (Oliphant et al., 2007).

An untagged form of ZIKV DIII (strain H/PF/2013, residues 299 to 407) was cloned into the pET21a vector (Novagen) and expressed by IPTG-induction in BL21 (DE3) bacterial cells (Agilent). Isolated inclusion bodies were solubilized and oxidatively re-folded, as previously described for WNV DIII (Nybakken et al., 2005). ZV-48 scFv was engineered with a (GGGS)₃ linker between the V_L and V_H domains, cloned into the pET21a vector, and expressed in the BL21 (DE3) as inclusion bodies. The ZV-48 scFv was refolded *in vitro* in a manner similar to ZIKV DIII. After protein A affinity purification, the ZV-2, ZV-64 and ZV-67 IgG were cleaved with immobilized papain (Pierce Biotechnology), and Fab fragments were recovered by passage

over a second protein A affinity column to remove cleaved Fc and any uncleaved IgG. The V_H and V_L of mAbs were amplified from hybridoma cell RNA by a 5' RACE procedure, and PCR products were sequenced as described (Tiller et al., 2009). The final sequences of mAbs were determined by combining PCR sequence results with our interpretation of the high-resolution electron density maps of the mAb-DIII complexes. The ZV-48 scFvs were complexed with excess DIII and purified by size exclusion chromatography in 150 mM NaCl and 20 mM HEPES pH 7.5. The ZV-48 scFv-DIII complexes were crystallized by hanging drop vapor diffusion at 14 mg/ml in 0.2 M Ammonium sulfate and 15 %(w/v) PEG 4000. Crystals were cryo-protected in a solution containing 20% ethylene-glycol and cooled in liquid nitrogen for data collection. Concentrated Fab and DIII preparations were mixed at a 1:1 stoichiometry, incubated at 4°C overnight, then used for crystallization trials without further purification. Diffraction-quality crystals of ZV-2-DIII complex were obtained in 0.1 M MES pH 6.5, 0.6 M NaCl and 20.6% PEG 4000 at 13 mg/ml. Diffraction-quality crystals of ZV-64-DIII were obtained in 0.1 M sodium acetate and 22% PEG 4000 at 15 mg/ml. Diffraction-quality crystals of ZV-67-DIII were obtained in 0.2 M Ammonium formate, 20% PEG 3350 at 14 mg/ml.

Structure determination and refinement. Fine-sliced diffraction data were collected at ALS beamline 4.2.2 (Molecular Biology Consortium) at 100 K at a wavelength of 1.0 Å using a CMOS detector in shutter-less mode. Data were processed in XDS (Kabsch, 2010) and scaled using AIMLESS (Evans and Murshudov, 2013). Molecular replacement phasing was accomplished in PHENIX (Adams et al., 2010) using the Phaser GUI (McCoy et al., 2007), with the structure of ZV-2 in complex with ZIKV DIII (H/PF/2013) determined first using the coordinates of WNV E16-DIII (RCSB:1ZTX) (Nybakken et al., 2005) assembled as three probes ($V_L V_H$, $C_L C_H$, and DIII) and subsequent structures determined using ZV-2-DIII coordinates. Cycles of model building and atomic refinement were carried out in COOT (Emsley et al., 2010) and PHENIX. A summary of data collection and refinement statistics is provided in **Table S1**.

Structural analysis. Antibody-antigen contacts were assessed using HBPLUS

employing default settings (McDonald and Thornton, 1994), buried surfaces were calculated using AREAIMOL (Lee and Richards, 1971), and shape complementarity was measured using Sc (Lawrence and Colman, 1993). All structural representations were colored and rendered using the PyMOL Molecular Graphics System (<http://www.pymol.org>).

Table S1. Data Collection and Refinement Statistics

	ZV-2 Fab-DIII complex	ZV-48 scFv-DIII complex	ZV-64 Fab-DIII complex	ZV-67 Fab-DIII complex
PDB ID code				
Unit-cell, Å	39.02, 113.44, 132.97	63.24, 87.98, 147.52	59.68, 92.16, 96.25	73.11, 82.93, 93.26
Space group	P2 ₁ 2 ₁ 2 ₁	C222 ₁	P2 ₁ 2 ₁ 2 ₁	P2 ₁ 2 ₁ 2 ₁
^a Resolution range, Å	33.65 - 1.65 (1.71 - 1.65)	48.5 - 1.70 (1.76 - 1.70)	19.63 - 1.40 (1.45 - 1.40)	57.54 - 1.40 (1.45 - 1.40)
Total reflections	479367 (47934)	645120 (57943)	1093004 (103810)	3080888 (292949)
Unique reflections	71306 (7038)	44589 (4335)	104933 (10362)	111954 (11045)
Average multiplicity	6.7 (6.8)	14.5 (13.3)	10.4 (10.0)	27.5 (26.5)
Mean I/σ(I)	18.78 (2.12)	14.28 (1.60)	19.70 (1.83)	22.62 (2.13)
Completeness, %	99 (99)	98 (96)	100 (100)	100 (100)
Rmerge	0.0592 (0.9598)	0.1504 (1.9540)	0.0821 (1.4200)	0.1098 (1.7170)
Rmeas	0.0642 (1.0390)	0.1559 (2.0320)	0.0864 (1.4970)	0.1119 (1.7500)
CC1/2	0.999 (0.723)	0.999 (0.723)	0.999 (0.595)	1 (0.789)
CC*	1 (0.916)	1 (0.916)	1 (0.864)	1 (0.939)
Refinement				
Rwork	0.1901 (0.2747)	0.1870 (0.3100)	0.1538 (0.2458)	0.1489 (0.1973)
^b Rfree	0.2214 (0.2916)	0.2134 (0.3361)	0.1866 (0.3038)	0.1794 (0.2519)
CC(work)	0.967 (0.789)	0.963 (0.844)	0.970 (0.826)	0.971 (0.906)
CC(free)	0.949 (0.727)	0.964 (0.725)	0.963 (0.726)	0.964 (0.843)
Number of Atoms				
non-hydrogen atoms	4961	3210	4911	5121
macromolecules	4253	2554	4205	4109
ligands	18	39	30	2
Protein residues	550	331	546	540
Solvent molecules	690	619	675	1009
RMS(bonds)	0.004	0.003	0.005	0.006
RMS(angles)	0.76	0.67	0.85	0.94
Coordinate Error (MLH)	0.21	0.21	0.16	0.13
Ramachandran, favored, %	98	98	98	99
Ramachandran, allowed, %	2.00	1.90	1.50	0.97
Ramachandran, outliers, %	0	0	0	0
Rotamer outliers, %	0.41	0	0.41	0.22
Clashscore	2.72	3.33	2.99	1.36
B-factor Model	25 TLS groups	26 TLS groups	anisotropic	anisotropic
Average B factor, Å²	31.68	29.48	21.45	20.94
macromolecules	30.56	25.98	19.50	17.98
ligands	34.31	73.38	33.71	20.45
solvent	38.55	41.19	33.06	32.97

^aValues in parentheses refer to the highest resolution shell. ^bR_{free} = free R factor based on random 5% of all data. Diffraction source was ALS BL4.2.2 using detector RDI CMOS_8M. Data processing, scaling statistics, and refinement statistics are described in the Experimental Procedures.

Table S2. Van der Waals contacts for Fab and scFv DIII complexes

DIII	ZV-2	DIII	ZV-67
Lys ^{E301}	Ile ^{H30} (1)	Thr ^{E309}	Tyr ^{H32} (4)
Thr ^{E315}	Ser ^{L56} (1)	Ala ^{E310}	Asn ^{H96} (3),Tyr ^{H32} (1)
Lys ^{E316}	Tyr ^{H100A} (12),Asp ^{H101} (1)	Ala ^{E311}	Asn ^{H96} (7),Tyr ^{H97} (2)
Ile ^{E317}	Tyr ^{H100A} (3)	Phe ^{E312}	Ser ^{L50} (1)
Pro ^{E318}	Tyr ^{H100A} (2)	Thr ^{E313}	Ser ^{L50} (3),Tyr ^{H97} (2)
Ala ^{E319}	Tyr ^{H100A} (3),Tyr ^{H100} (3)	Phe ^{E314}	Thr ^{L31} (1)
Glu ^{E320}	Asn ^{L30D} (4),Tyr ^{H100} (2)	Gln ^{E331}	Tyr ^{H97} (3)
Thr ^{E321}	Asn ^{L30D} (5),Gly ^{H98} (3)	Tyr ^{E332}	Tyr ^{H97} (5)
Leu ^{E322}	His ^{L30A} (4),Tyr ^{L32} (1),Asn ^{L30D} (1),Gly ^{L30C} (1)	Ala ^{E333}	Tyr ^{H97} (13),Asn ^{H96} (1)
Thr ^{E327}	Tyr ^{H100A} (2),Tyr ^{H96} (1),Ser ^{H99} (1)	Gly ^{E334}	Ser ^{H31} (2)
Glu ^{E329}	Tyr ^{H32} (5),Arg ^{H94} (5)	Thr ^{E335}	Ser ^{H31} (7),Thr ^{H30} (4),Tyr ^{H52} (1) Ara ^{H53} (5.),Tvr ^{H32} (1)
Asn ^{E362}	Ile ^{H30} (3)	Asp ^{E336}	Ser ^{H31} (2)
Val ^{E364}	Thr ^{H28} (4)	Gly ^{E337}	Arg ^{H53} (1)
Ile ^{E365}	Thr ^{H28} (1)	Ser ^{E368}	Arg ^{H53} (3)
Thr ^{E366}	Thr ^{H28} (3)	Glu ^{E370}	Tyr ^{L94} (1),Tyr ^{H52} (6),Asn ^{H56} (4), Tyr ^{H58} (5)
Glu ^{E367}	Gly ^{H26} (8),Tyr ^{H27} (3),Ser ^{H25} (3)	Asn ^{E371}	Tyr ^{L94} (3),Tyr ^{L96} (3), Tyr ^{H97} (6)
Ser ^{E372}	Gly ^{H26} (4),Tyr ^{H27} (3)	Glu ^{E393}	Tyr ^{L49} (4),Tyr ^{L55} (4),Thr ^{L56} (4)
Lys ^{E373}	Tyr ^{H32} (1),Val ^{H2} (1),Gly ^{H26} (1), Tyr ^{H27} (4),Thr ^{H28} (2),Tyr ^{H102} (1)	Lys ^{E394}	Leu ^{L46} (1),Tyr ^{L49} (11) Asn ^{H96} (5),Gly ^{H98} (3)
Met ^{E374}	Tyr ^{H32} (4),Thr ^{H28} (1)	Lys ^{E395}	Tyr ^{L49} (5)
Met ^{E375}	Tyr ^{H32} (5),Tyr ^{H96} (4),Tyr ^{H100A} (2)	Ile ^{E396}	Asn ^{L53} (3)
Glu ^{E377}	Tyr ^{H96} (5)	Thr ^{E397}	Asn ^{L53} (2)
DIII	ZV-48	DIII	ZV-64
Leu ^{E307}	Asn ^{L30C} (1),Asn ^{L30D} (1),Glu ^{L30E} (5)	Leu ^{E307}	Asn ^{L30D} (3),Gln ^{L30E} (3),Ser ^{L30C} (1)
Lys ^{E340}	Ser ^{L30B} (3),Asn ^{L30C} (1),Glu ^{L30E} (5)	Lys ^{E340}	Ser ^{L30B} (3)
Pro ^{E342}	Asn ^{L30C} (1)	Pro ^{E342}	Ser ^{L30C} (2)
Ala ^{E343}	Asn ^{L30C} (3)	Ala ^{E343}	Ser ^{L30C} (5)
Gln ^{E344}	Tyr ^{L30A} (2),Asn ^{L30D} (1), Tyr ^{L32} (1)	Gln ^{E344}	Tyr ^{L30A} (2),Asn ^{L30D} (1),Tyr ^{L32} (1)
Val ^{E347}	Tyr ^{L94} (1.)Trp ^{H33} (4), Met ^{H50} (1)	Val ^{E347}	Tyr ^{L94} (1),Trp ^{H33} (4),Met ^{H50} (1)
Asp ^{E348}	Trp ^{H33} (6)	Asp ^{E348}	Tyr ^{L94} (1),Trp ^{H33} (8),His ^{H35} (1)
Gln ^{E350}	Tyr ^{H32} (1), Arg ^{H94} (1),Leu ^{H95} (4) , Gly ^{H96} (4), Asn ^{H97} (4),Met ^{H99} (6)	Gln ^{E350}	Ser ^{H31} (1),Tyr ^{H95} (1), Tyr ^{H96} (2), Tyr ^{H97} (5)
Thr ^{E351}	Tyr ^{L32} (1),Trp ^{L50} (1),Tyr ^{L91} (2), Tyr ^{L96} (3),Leu ^{H95} (1),Gly ^{H96} (1), Asn ^{H97} (3)	Thr ^{E351}	Tyr ^{L32} (1), Trp ^{L50} (2),Tyr ^{L91} (2), Tyr ^{L96} (3),Tyr ^{H97} (1)
Leu ^{E352}	Tyr ^{L32} (6)	Leu ^{E352}	Tyr ^{L32} (6)
Thr ^{E353}	Tyr ^{L32} (2), Tyr ^{L91} (6), Tyr ^{L92} (2), Tyr ^{L94} (4), Tyr ^{L96} (4)	Thr ^{E353}	Tyr ^{L32} (2),Tyr ^{L91} (5),Tyr ^{L92} (2), Tyr ^{L94} (4),Tyr ^{L96} (4)
Pro ^{E354}	Tyr ^{L30A} (10) ,Tyr ^{L32} (1),Tyr ^{L92} (1)	Pro ^{E354}	Tyr ^{L30} (1),Tyr ^{L30A} (5),Tyr ^{L92} (1)
Leu ^{E358}	Asn ^{L30C} (1)	Val ^{E355}	Tyr ^{L94} (1)
Asp ^{E384}	Asn ^{H56} (4)	Leu ^{E358}	Ser ^{L30C} (1)
Tyr ^{E386}	Asn ^{H31} (1)	Val ^{E391}	Asn ^{L30D} (1),Lys ^{L30F} (1)

Van der Waals contacts summary										
	CDR-H1 26-32	CDR-H2 52-56	CDR-H3 95-102	FRM-H	Total V_H	CDR-L1 24-34	CDR-L2 50-56	CDR-L3 89-97	FRM-L	Total V_L
ZV-2	56	0	45	6	107	16	1	0	0	17
ZV-48	2	4	23	12	41	46	1	23	0	70
ZV-64	1	0	9	14	24	39	2	24	0	65
ZV-67	21	20	50	5	96	1	17	7	21	46

Summary of van der Waals contacts across the interface in different mAb-DIII complexes. The amino acids are labeled (in superscript) to indicate their specific positions in the heavy chain (H), light chain (L) or DIII (E) sequences. Interactions were determined using HBPLUS (McDonald, 1994) using a cutoff distance of 3.9 Å.

Table S3. Hydrogen bond contacts for Fab and scFv DIII complexes with DIII

Direct hydrogen bonds			
DIII	ZV-2	DIII	ZV-67
Ile ^{E317} (O)	Tyr ^{H100A} (OH)	Ala ^{E311} (N)	Asn ^{H96} (OD1)
Glu ^{E320} (O)	Asn ^{L30D} (ND2)	Thr ^{E313} (OG1)	Ser ^{L50} (OG)
Thr ^{E327} (O)	Tyr ^{H100A} (OH)	Thr ^{E335} (O)	Arg ^{H53} (NH1)
Glu ^{E329} (OE2)	Tyr ^{H32} (OH), Arg ^{H94} (NH1)	Thr ^{E335} (N)	Ser ^{H31} (O)
Val ^{E364} (O)	Thr ^{H28} (OG1)	Thr ^{E335} (OG1)	Thr ^{H30} (O)
Glu ^{E367} (OE2)	Gly ^{H26} (N)	Asn ^{E371} (ND2)	Tyr ^{L94} (OH)
Lys ^{E373} (NZ)	Tyr ^{H102} (OH)	Gly ^{E337} (O)	Arg ^{H53} (NH1)
Lys ^{E373} (N)	Gly ^{H26} (O)	Glu ^{E370} (OE2)	Asn ^{H56} (ND2), Tyr ^{H58} (OH)
Lys ^{E373} (O)	Thr ^{H28} (N)	Asn ^{E371} (OD1)	Tyr ^{H97} (OH)
Glu ^{E377} (OE1)	Tyr ^{H96} (OH)	Lys ^{E394} (NZ)	Asn ^{H96} (O), Gly ^{H98} (O)
		Lys ^{E395} (O)	Tyr ^{L49} (OH)
		Thr ^{E397} (N)	Asn ^{L53} (OD1)
Indirect (solvent mediated) hydrogen bonds			
DIII	ZV-2	DIII	ZV-67
Thr ^{E315} (O)	Ser ^{L56} (OG)	Thr ^{E313} (OG1)	Ser ^{L5} (OG)
Lys ^{E316} (O)	Tyr ^{H100A} (OH)	Phe ^{E314} (O)	Thr ^{L31} (OG1)
Ile ^{E317} (O)	Tyr ^{L49} (OH)	Gln ^{E331} (OE1)	Phe ^{L91} (O)
Glu ^{E320} (OE2)	Gly ^{L30C} (O)	Ala ^{E333} (O)	Glu ^{H95} (O)
Thr ^{E366} (OG1)	Tyr ^{H27} (O)	Thr ^{E335} (OG1)	Ser ^{L43} (O)
Asn ^{E371} (O)	Gly ^{H26} (O)	Glu ^{E370} (OE1)	Ser ^{H54} (OG)
Ser ^{E372} (OG)	Thr ^{H28} (OG1)	Asn ^{E371} (OD1)	Tyr ^{H52} (OH)
Met ^{E375} (O)	Tyr ^{H96} (OH)	Thr ^{E397} (OG1) Thr ^{E397} (O)	Ser ^{L52} (OG), Asn ^{L53} (OD1)
Glu ^{E377} (OE1)	Tyr ^{H97} (O)		

Direct hydrogen bonds			
DIII	ZV-48	DIII	ZV-64
Lys ^{E340} (NZ)	Ser ^{L30B} (O), Glu ^{L30E} (OE2)	Lys ^{E340} (NZ)	Ser ^{L30B} (O)
Ala ^{E343} (O)	Asn ^{L30C} (ND2)	Ala ^{E343} (N)	Ser ^{L30C} (OG)
Gln ^{E344} (OE1)	Asn ^{L30D} (ND2)	Ala ^{E343} (O)	Ser ^{L30C} (OG)
Val ^{E347} (O)	Trp ^{H33} (NE1)	Val ^{E347} (O)	Trp ^{H33} (NE1)
Gln ^{E350} (NE2)	Gly ^{H96} (O), Met ^{H99} (O)	Gln ^{E350} (O)	Tyr ^{H97} (N)
Gln ^{E350} (O)	Asn ^{H97} (ND2)	Thr ^{E351} (OG1)	Tyr ^{L96} (OH)
Thr ^{E351} (OG1)	Tyr ^{L96} (OH)	Leu ^{E352} (O)	Tyr ^{L32} (OH)
Leu ^{E352} (O)	Tyr ^{L32} (OH)	Thr ^{E353} (OG1)	Tyr ^{L91} (O), Tyr ^{L96} (OH)
Thr ^{E353} (OG1)	Tyr ^{L96} (OH), Tyr ^{L91} (O)		
Asp ^{E384} (OD2)	Asn ^{H56} (ND2)		

Indirect (solvent mediated) hydrogen bonds			
DIII	ZV-48	DIII	ZV-64
Tyr ^{E305} (O)	Glu ^{L30E} (OE2)	Val ^{E341} (O)	Ser ^{L30C} (OG)
Val ^{E341} (O)	Asn ^{L30C} (O)	Asp ^{E348} (OD2)	His ^{H35} (NE2)
Asp ^{E348} (OD2)	His ^{H35} (NE2)	Met ^{E349} (O)	Tyr ^{H97} (O)
Gln ^{E350} (OE1)	Trp ^{H33} (O)	Asp ^{E348} (OD2), Thr ^{E351} (OG1)	Tyr ^{L94} (OH),Tyr ^{L96} (OH)
Thr ^{E351} (OG1)	Tyr ^{L94} (OH),Tyr ^{L96} (OH)	Thr ^{E353} (O)	Tyr ^{L94} (OH)
Thr ^{E353} (O)	Tyr ^{L94} (OH)	Pro ^{E354} (O)	Tyr ^{L92} (O)
Pro ^{E354} (O)	Tyr ^{L92} (O)	Val ^{E355} (O)	Tyr ^{L30A} (OH)
Val ^{E355} (O)	Tyr ^{L30A} (OH)	Asp ^{E384} (O)	Ser ^{H56} (OG)
Tyr ^{E386} (OH)	Asn ^{H31} (O)		

Hydrogen bonds summary										
	CDR-H1 26-32	CDR-H2 52-56	CDR-H3 95-102	FRM- H	Total V _H	CDR-L1 24-34	CDR-L2 50-56	CDR-L3 89-97	FRM-L	Total V _L
ZV-2	5+3	0+0	4+3	1+0	16	1+1	0+1	0+0	0+1	4
ZV-48	0+1	1+0	3+0	1+2	8	5+3	0+0	3+4	0	15
ZV-64	0+0	0+1	1+1	1+1	5	4+2	0+0	3+4	0	13
ZV-67	2+0	3+2	4+1	1+0	13	0+1	2+2	1+1	1+2	10

Summary of hydrogen bonding across the interface in different mAb-DIII complexes. The amino acids are labeled (in superscript) to indicate their specific positions in the heavy chain (H), light chain (L) or DIII (E) sequences. Hydrogen bonding interactions were assessed using HBPLUS (McDonald, 1994).

Table S4. MAb-DIII contacts and buried surface area summary

	Van der Waals contacts	Hydrogen bonds	Buried Surface Area (\AA^2) at the mAbs/DIII Interface			Buried Surface Area (\AA^2) at the DIII/ mAbs Interface		
	V_H+V_L Total	V_H+V_L Total	V_H	V_L	V_H+V_L Total	DIII Total	DIII surface lost (%)	Sc
ZV-2	124	20	800	234	943	876	14.3	0.676
ZV-48	111	23	313	542	767	875	14.6	0.689
ZV-64	89	18	306	522	750	829	14.1	0.708
ZV-67	142	23	580	410	866	882	13.6	0.703

For each antibody, the total number of van der Waals contacts and direct and water-mediated hydrogen bonds are listed (as from **Tables S2 and S3**), as is the amount of surface area buried when bound to DIII. The surface area lost by either antibody chain alone (V_H or V_L) is given separately for comparison. The total area buried by both antibody chains due to interaction with DIII is also given (V_H or V_L Total). The amount of surface area lost by DIII due to interaction with antibody is given (DIII Total). The same value is given as a percent of the entire DIII surface area. All area values were calculated from the structural models using the program areaimol (Lee, 1971). The shape complementarity (Sc) at each mAb-DIII interface was calculated from the structural models using the program SC (Lawrence, 1993). Interfaces that mesh precisely have an Sc value of 1.

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